



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 12:00 AM UTC

PDB ID : 7XHN / pdb_00007xhn
EMDB ID : EMD-33196
Title : Structure of human inner kinetochore CCAN-DNA complex
Authors : Sun, L.F.; Tian, T.; Wang, C.L.; Yang, Z.S.; Zang, J.Y.
Deposited on : 2022-04-09
Resolution : 3.71 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

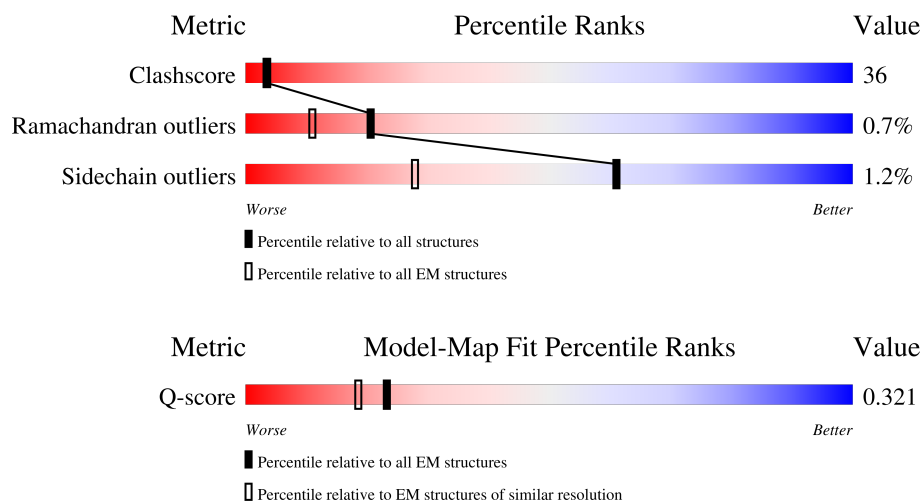
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



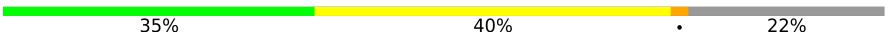
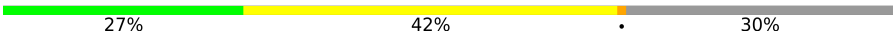
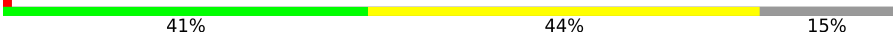
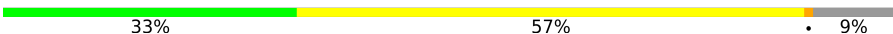
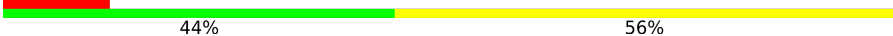
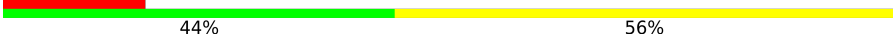
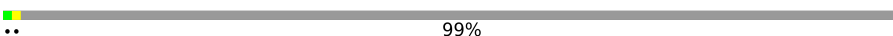
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10534 (3.21 - 4.21)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	300	
1	o	300	
2	H	253	
3	I	756	

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Mol	Chain	Length	Quality of chain
4	K	269	
5	L	344	
6	M	180	
7	N	345	
8	P	288	
9	S	138	
10	T	561	
11	W	88	
12	X	81	
13	G	25	
14	J	25	
15	C	943	
15	c	943	
16	Q	274	
17	U	418	
18	R	177	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 23364 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	o	12	Total	C	N	O		0	0
			95	59	18	18			
1	O	206	Total	C	N	O	S	0	0
			1588	1017	269	294	8		

- Molecule 2 is a protein called Centromere protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	195	Total	C	N	O	S	0	0
			1560	980	273	299	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	248	HIS	-	expression tag	UNP Q9H3R5
H	249	HIS	-	expression tag	UNP Q9H3R5
H	250	HIS	-	expression tag	UNP Q9H3R5
H	251	HIS	-	expression tag	UNP Q9H3R5
H	252	HIS	-	expression tag	UNP Q9H3R5
H	253	HIS	-	expression tag	UNP Q9H3R5

- Molecule 3 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	517	Total	C	N	O	S	0	0
			4111	2700	661	724	26		

- Molecule 4 is a protein called Centromere protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	230	Total	C	N	O	S	0	0
			1869	1183	312	364	10		

- Molecule 5 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	302	Total	C	N	O	S	0	0
			2422	1576	396	436	14		

- Molecule 6 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	168	Total	C	N	O	S	0	0
			1298	825	232	234	7		

- Molecule 7 is a protein called Centromere protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	305	Total	C	N	O	S	0	0
			2493	1601	434	448	10		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	340	HIS	-	expression tag	UNP Q96H22
N	341	HIS	-	expression tag	UNP Q96H22
N	342	HIS	-	expression tag	UNP Q96H22
N	343	HIS	-	expression tag	UNP Q96H22
N	344	HIS	-	expression tag	UNP Q96H22
N	345	HIS	-	expression tag	UNP Q96H22

- Molecule 8 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	224	Total	C	N	O	S	0	0
			1808	1144	311	344	9		

- Molecule 9 is a protein called Centromere protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	97	Total	C	N	O	S	0	0
			790	494	141	150	5		

- Molecule 10 is a protein called Centromere protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	99	Total	C	N	O	S	0	0
			804	516	139	142	7		

- Molecule 11 is a protein called CENP-W.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	75	Total	C	N	O	S	0	0
			584	367	119	95	3		

- Molecule 12 is a protein called Centromere protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	74	Total	C	N	O	S	0	0
			590	378	104	107	1		

- Molecule 13 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	25	Total	C	N	O	P	0	0
			513	241	98	149	25		

- Molecule 14 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	25	Total	C	N	O	P	0	0
			512	241	95	151	25		

- Molecule 15 is a protein called Centromere protein C.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	C	5	Total	C	N	O	0	0
			40	28	5	7		
15	c	13	Total	C	N	O	0	0
			105	69	17	19		

- Molecule 16 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	164	Total	C	N	O	S	0	0
			1175	718	207	242	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	269	HIS	-	expression tag	UNP Q7L2Z9
Q	270	HIS	-	expression tag	UNP Q7L2Z9
Q	271	HIS	-	expression tag	UNP Q7L2Z9
Q	272	HIS	-	expression tag	UNP Q7L2Z9
Q	273	HIS	-	expression tag	UNP Q7L2Z9
Q	274	HIS	-	expression tag	UNP Q7L2Z9

- Molecule 17 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	U	140	Total	C	N	O	0	0
			699	419	140	140		

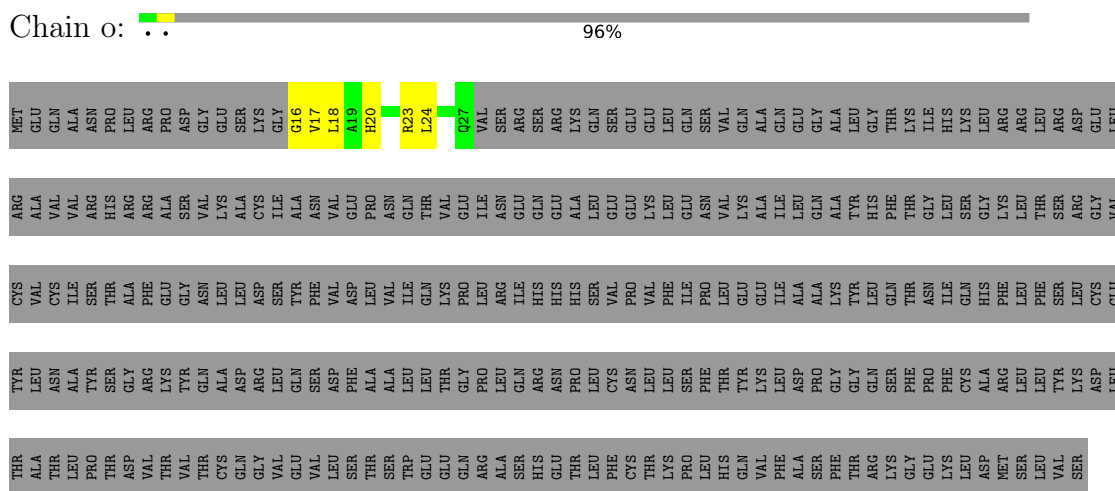
- Molecule 18 is a protein called Centromere protein R.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	62	Total	C	N	O	0	0
			308	184	62	62		

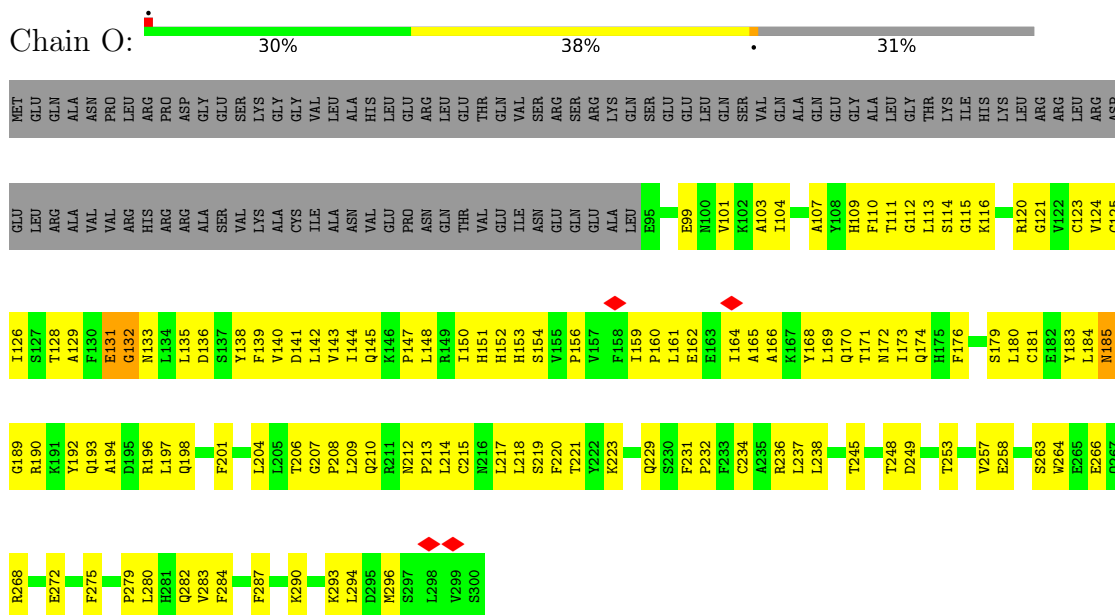
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Centromere protein O



• Molecule 1: Centromere protein O



• Molecule 2: Centromere protein H

K207	E135	K67	MET
K208	L136	THR	GLU
T209	N137	P80	GLU
T210	K138	GLN	GLN
V211	L139	GLN	PRO
	I140	ILE	GLN
V215	M141	MET	MET
F216	K142	GLN	GLN
K217	S143	ASP	ASP
N218	Q144	K76	ALA
L219	Q145	Q77	ASP
I220	E146	I78	GLU
	E147	E79	PRO
V225	M148	A80	ALA
N226	D149	K81	ASP
V227	L150	I82	SER
		E83	GLY
P231	L154	D84	GLY
A232	L155	L85	GLU
L233	D156	E86	GLY
	I157	N87	ARG
V237	R158	E88	ALA
L238	K159	I89	GLY
	V160	E90	GLY
E241	R161	E91	PRO
LYS	L162	V92	PRO
ASN	Q163	K93	GLN
VAL	L164	V94	VAL
ASP	K165	A95	ALA
MET	Q166	F96	GLY
MET	A167		ALA
HIS	S168	K99	GLN
HIS		K100	ALA
HIS	K171	L101	ALA
HIS	L172	A102	CYS
HIS	L173		SER
HIS	E174	R105	GLU
HIS	I175	M106	ASP
	Q176	R107	
	T177		R39
	E178	L112	L42
	K179	K113	L43
	N180	K114	L44
	K183	N115	R45
	I184	L116	L46
	D185	E117	R47
	L186	K118	A48
	D187		Q49
	S188	R121	
	E189	S124	Q52
	E190	V125	Q53
		L126	L54
	I197	M127	L55
	L198		E56
		M130	V57
		K131	K58
	L201	H132	S59
	L202	L133	M60
		L134	V61
	L206		

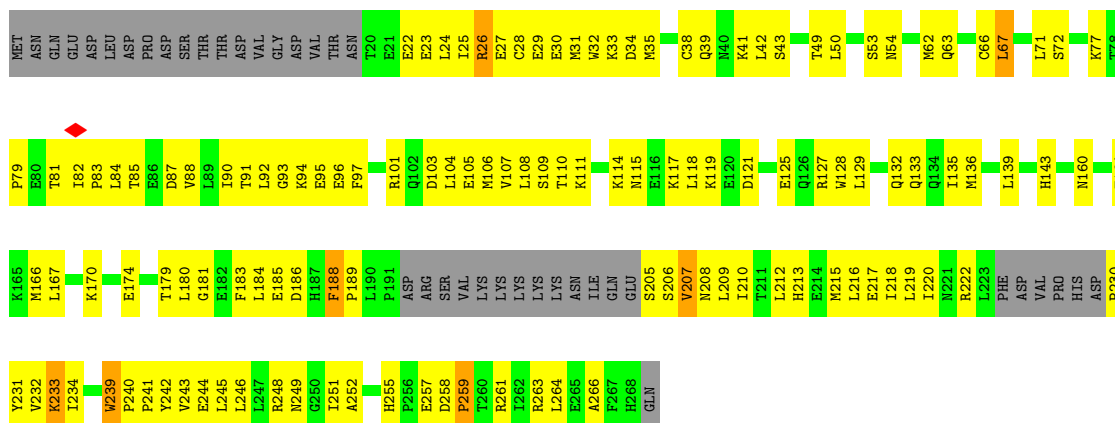
Chain I: 31% 36% 32%

TRP	F583	SER	L449	GLU	ARG	Y200	K131	ALA	MET
THR	P584	PRO	C450	LEU	PRO	V201	C132	E62	SER
LYS	I587	LEU	C451	PRO	LEU	C202	M133	E63	PRO
PRO	F588	GLU	R452	SER	ARG	H203	T134	D64	GLN
PHE	Y589	THR	S453	GLN	ARG	L204	P135	A65	LYS
GLN	S590	THR		MET	LYS	L205	P136	L66	ARG
LYS	A591	GLY	Q457	GLY	TRP	T206	T137	Q67	VAL
GLY	L592	G527	L458	S365	LEU	V207	V138	M68	LYS
ILE	L593	M530	S460	L371	SER	L208	I139	ASN	ASN
TYR	S594	N531	S461	L371	LEU	T209	S140	G71	VAL
ILE	L595	S532	I462	Y375	SER	K210	E141	Y72	GLN
ASP	D596	V533	P463	I376	VAL		D142	F73	ALA
PRO	T597	S534	F464	N377	PRO	N213	S143	E74	GLN
GLU	S598	K535		C378	VAL		V144	G75	ASN
ILE	I599	L536		V379	LEU	V219	V145	K76	ARG
LEU	L600	I537	F467		ASN	H220	K146	F77	THR
GLU	M601	H538	K471	E382	SER	K221	A147	A80	SER
LYS	Q602	T539	P472		SER	L222	V148	S81	GLY
THR	L603	V540	L473	Y389	SER		S149	Q82	GLY
GLY		G541	L475	Y390	TYR	M229	W150	M83	SER
VAL	I606	W542	F476	W391	THR		L151	K84	SER
ALA	M607	L543	D476	L392	LYS	P233	C152	D85	PHE
GLU	H608	S544	H477		GLU	H234		K86	GLN
THR	R609	T545	L478	T395	CYS	L235	C156	T87	THR
LYS	Y610	T546	A479		GLY			L88	THR
ASN	R611	ASL	Q480	E399	LYS	L249	S159	E89	LEU
SER	K612	M548	L481	Y403	LYS	T250	T160	K90	SER
LEU	R613	R549	F482		GLU	S251	K161	H91	ALA
ASN	L614	L550	F483	Y403	MET	V252	L162	L92	TRP
VAL	T615	E551	T484	G411	SER		L163	K93	LYS
VAL		S552		K412	LEU	LEU	F164	T94	VAL
THR	K618	N553	I487		SER	PRO	Y165	E95	LYS
HIS	H619	L557	K490	N416	ASP	VAL	R166	E96	GLN
H685	P686	L558	C491	F417	CYS	ARG	W167		ASP
S687	E621			L418	LEU	LYS	L168	A99	PRO
F688	LEU	H559	L494	I421	ASN	LYS		W100	SER
L689	VAL	F560	Q495	I422	ARG	T260	M171	K101	ASN
GLN	S690	I561			SER		F172	N102	SER
LYS	Y691	L562			GLY	E266	D173	G103	SER
THR	D663	THR	K498	F427	SER		F174	L104	LYS
LYS	F564	LYS	E499	L428	PHE	K270	I175	A105	ASN
SER	Y565	LYS		Q429	PRO		D176	S106	LYS
GLY	E566	GLU	Q502	Q430	LEU	L273	R177	E107	SER
PHE	K567	GLU	N503	G431	GLU			I108	LYS
LEU	M631	GLN	F504	F432	GLN	P283	I181	I109	HIS
GLN	F632	LEU	L505	Y433	GLN	SER	M182	D110	GLN
GLU		D570	L506	S434	GLN	PRO	L183	T111	ASN
SER	T636	I571	W607	C435	SER	GLU	L184	L112	ASN
PRO	Y637	Y572	L508	E436	PHE	PRO	Y185	L113	PRO
GLU		I573	S509		PRO	LEU	C186		VAL
GLU	N641	I574	M510	Y440	GLN	LYS		L117	GLY
ARG	H642	Y575		K441	LEU	LEU	F189	ASP	ASP
THR	Y643	N576	H513	S442	LEU	MET		K120	TYR
VAL	L644		M514	L443	GLN	LEU	L192	F121	GLU
ASN		S578	K615	P444					



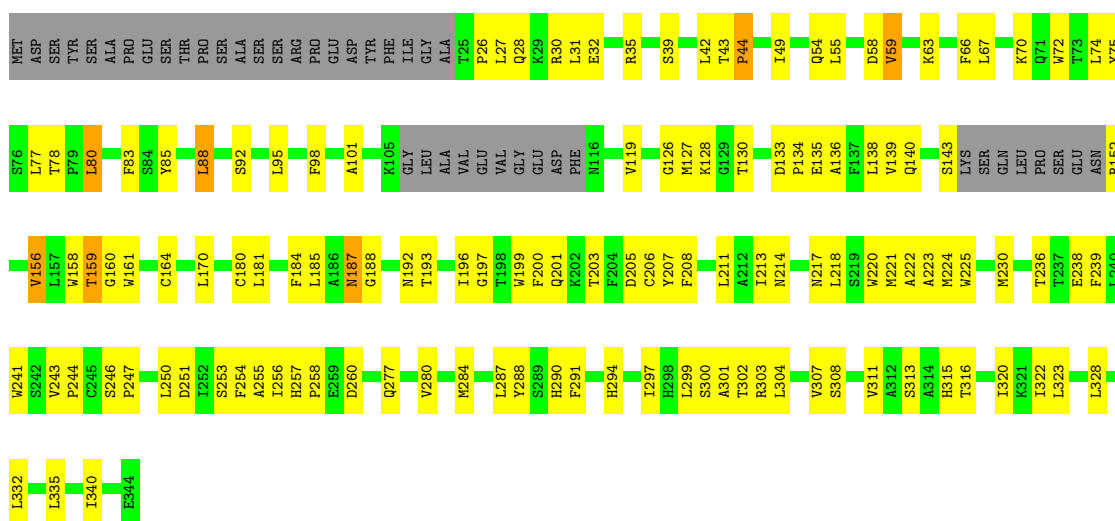
• Molecule 4: Centromere protein K

Chain K: 38% 45% 14%



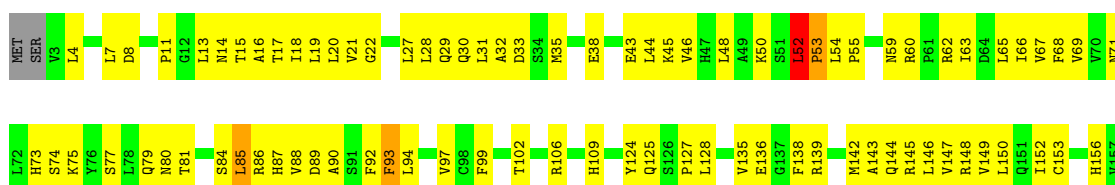
• Molecule 5: Centromere protein L

Chain L: 50% 35% 12%

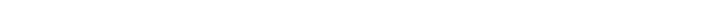


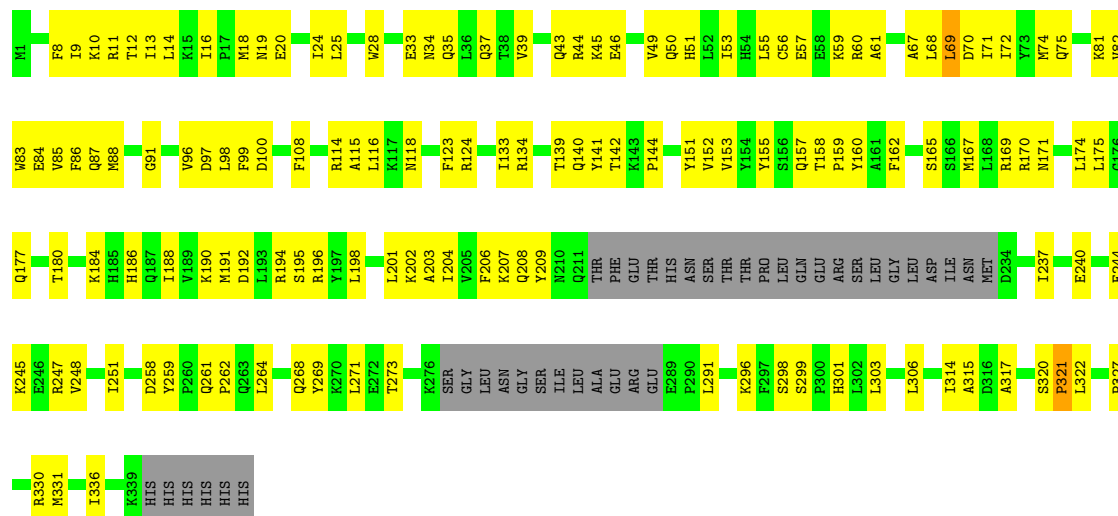
• Molecule 6: Centromere protein M

Chain M: 41% 50% 7%

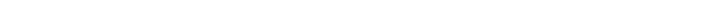


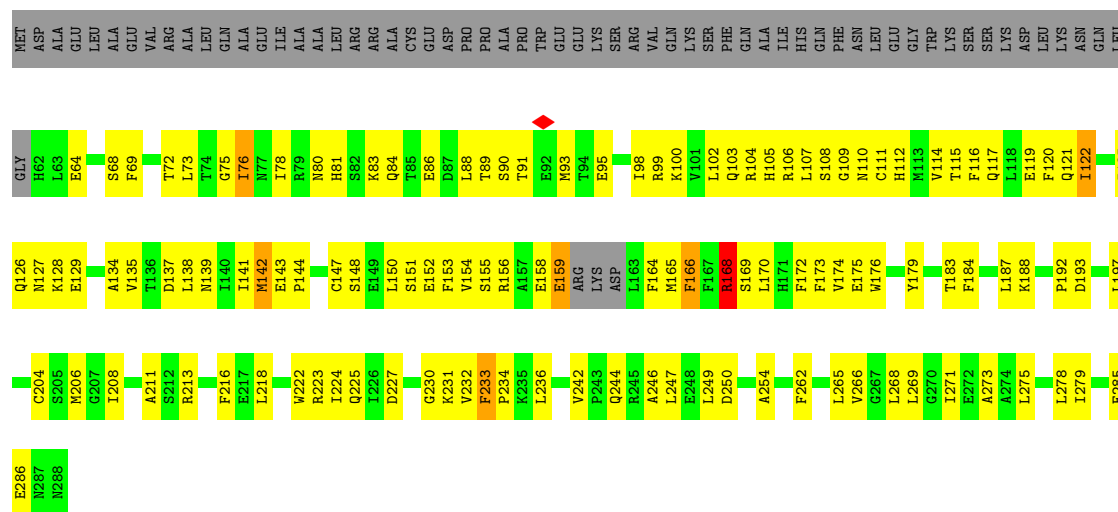
- Molecule 7: Centromere protein N

Chain N:  48% 39% 12%

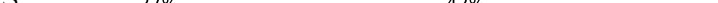


- Molecule 8: Centromere protein P

Chain P:  35% 40% . 22%

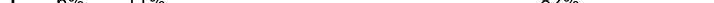


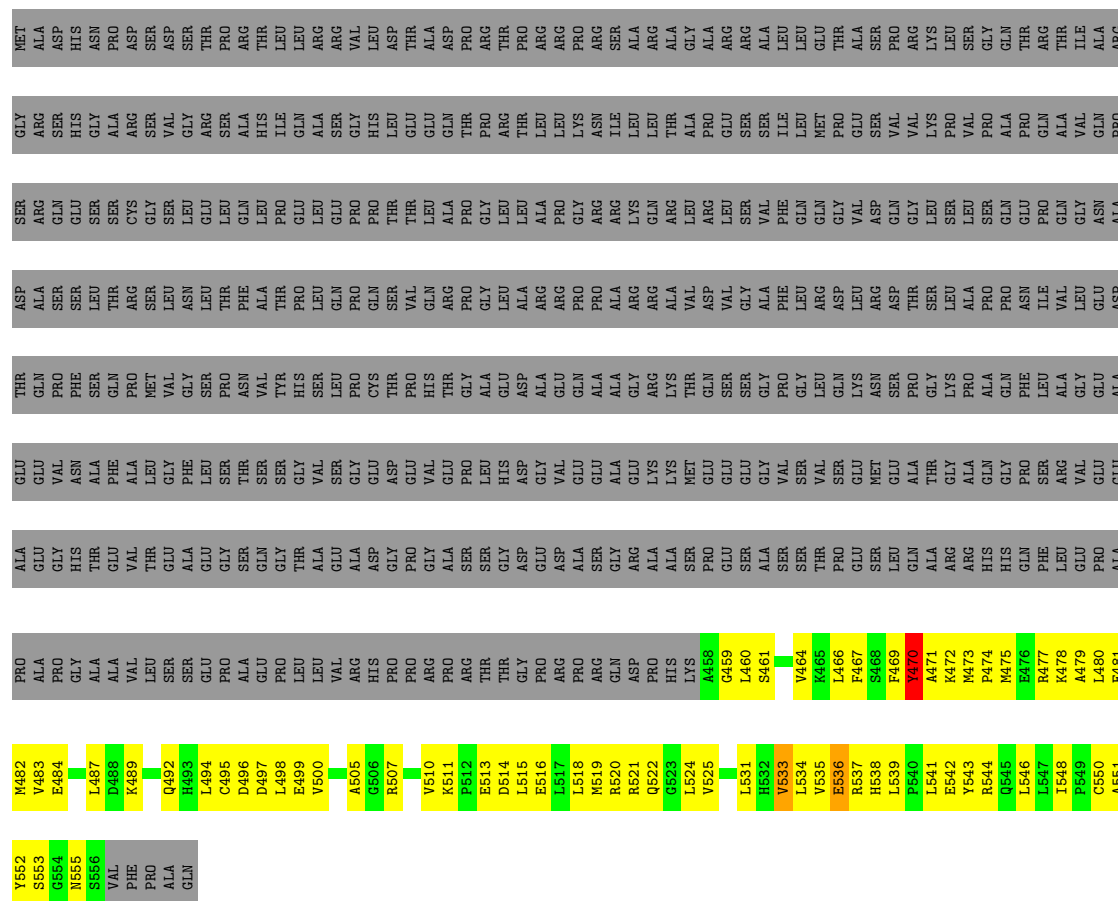
- Molecule 9: Centromere protein S

Chain S:  27% 42% 1% 30%

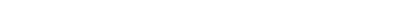


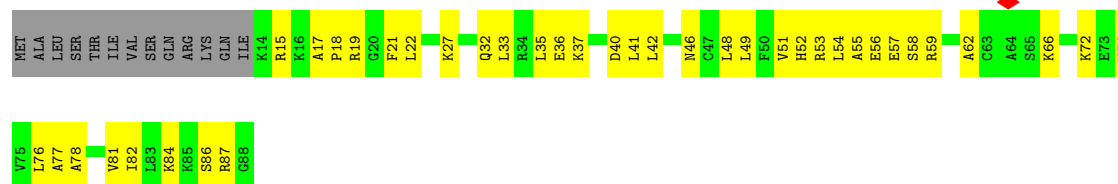
- Molecule 10: Centromere protein T

Chain T:  6% 11% 82%



- Molecule 11: CENP-W

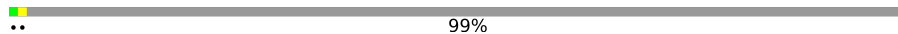
Chain W:  41% 44% 15%

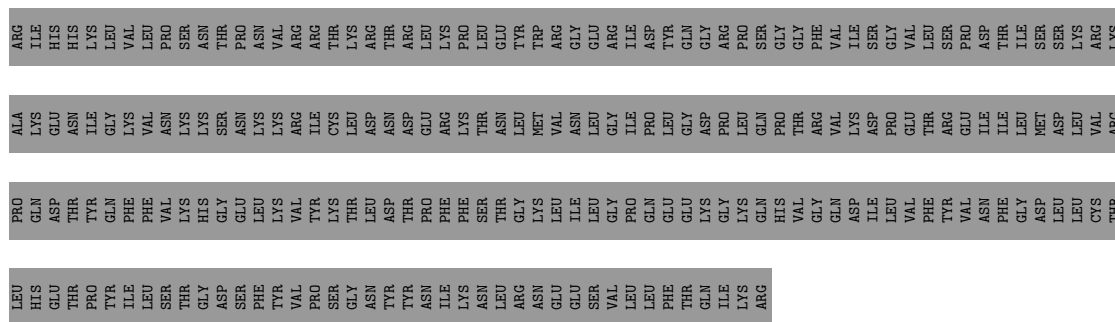


- Molecule 12: Centromere protein X

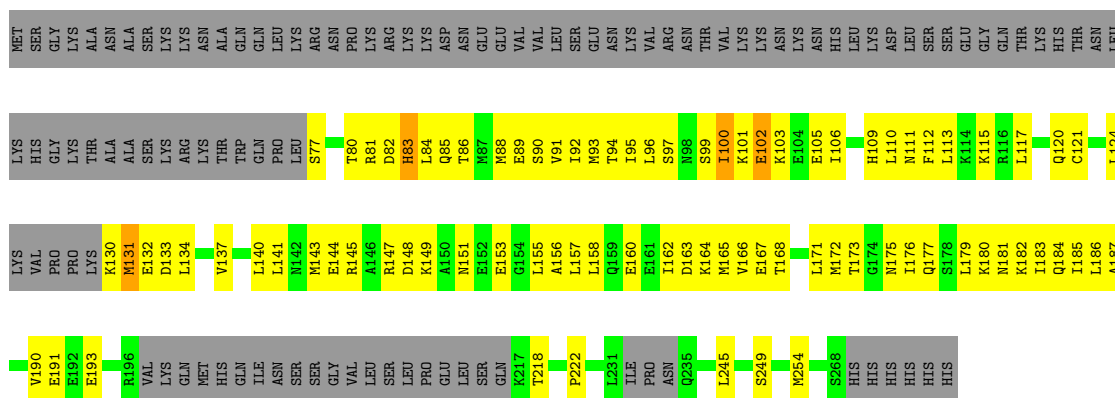
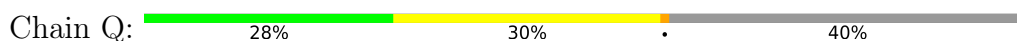
Chain X: 33% 57% 9%

- Molecule 15: Centromere protein C

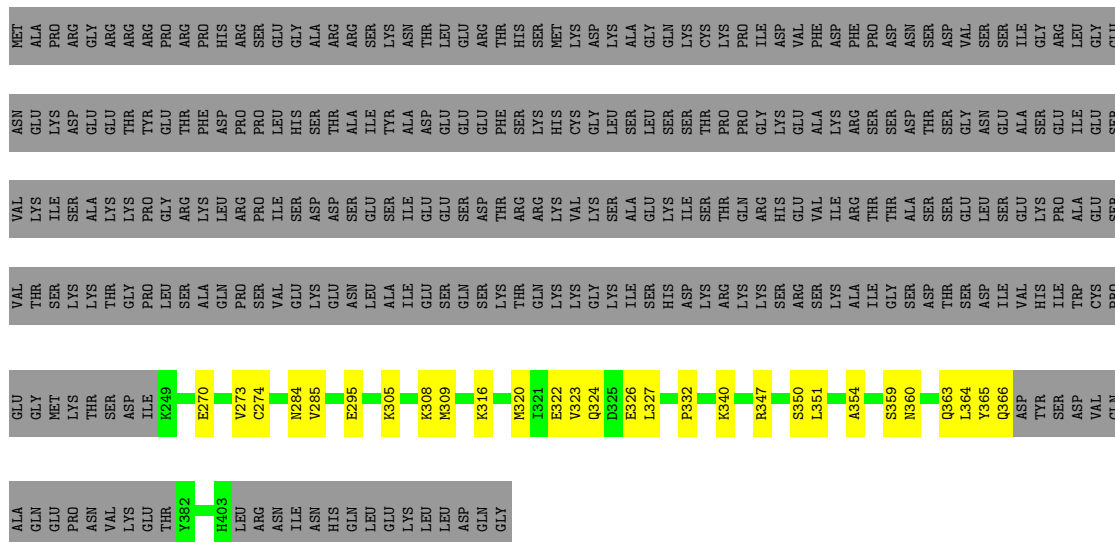
Chain c: [illegible]



- Molecule 16: Centromere protein Q



- Molecule 17: Centromere protein U



- Molecule 18: Centromere protein R





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79777	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.924	Depositor
Minimum map value	-2.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	380.64, 380.64, 380.64	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.22, 1.22, 1.22	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	O	0.84	7/1624 (0.4%)	1.21	9/2208 (0.4%)
1	o	0.23	0/95	0.50	0/127
2	H	0.36	0/1566	0.69	1/2093 (0.0%)
3	I	0.42	5/4210 (0.1%)	0.63	2/5704 (0.0%)
4	K	0.49	2/1897 (0.1%)	0.66	2/2558 (0.1%)
5	L	0.34	1/2487 (0.0%)	0.53	0/3379
6	M	0.59	2/1320 (0.2%)	0.68	2/1791 (0.1%)
7	N	0.24	0/2547	0.47	0/3440
8	P	0.46	2/1839 (0.1%)	0.66	4/2474 (0.2%)
9	S	0.32	0/799	0.70	2/1070 (0.2%)
10	T	0.46	2/821 (0.2%)	0.61	1/1105 (0.1%)
11	W	0.32	0/590	0.58	0/785
12	X	0.34	0/596	0.68	0/801
13	G	0.18	0/575	0.34	0/885
14	J	0.20	0/573	0.37	0/882
15	C	0.32	0/40	1.00	0/53
15	c	0.17	0/106	0.70	0/141
16	Q	0.39	1/1175 (0.1%)	0.70	1/1580 (0.1%)
17	U	0.26	0/697	0.68	3/972 (0.3%)
18	R	0.18	0/306	0.52	0/424
All	All	0.43	22/23863 (0.1%)	0.67	27/32472 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1
8	P	0	1
All	All	0	2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	208	PRO	CB-CG	18.97	2.44	1.49
4	K	259	PRO	CA-CB	14.73	1.62	1.53
1	O	208	PRO	CG-CD	-13.77	1.03	1.50
6	M	52	LEU	CG-CD2	-13.41	1.08	1.52
1	O	208	PRO	N-CA	-8.82	1.36	1.46

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	208	PRO	CB-CG-CD	-33.14	0.05	106.10
1	O	208	PRO	CA-N-CD	-21.41	82.02	112.00
6	M	53	PRO	CA-N-CD	-12.84	94.02	112.00
1	O	208	PRO	CA-CB-CG	-12.62	80.52	104.50
1	O	208	PRO	N-CD-CG	-12.45	84.53	103.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	47	ARG	Sidechain
8	P	168	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1588	0	1540	139	0
1	o	95	0	96	10	0
2	H	1560	0	1633	168	0
3	I	4111	0	4032	324	0
4	K	1869	0	1857	161	0
5	L	2422	0	2398	128	0
6	M	1298	0	1349	126	0
7	N	2493	0	2511	146	0
8	P	1808	0	1810	146	0
9	S	790	0	798	79	0
10	T	804	0	814	87	0
11	W	584	0	631	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	X	590	0	620	77	0
13	G	513	0	279	19	0
14	J	512	0	280	23	0
15	C	40	0	36	3	0
15	c	105	0	106	9	0
16	Q	1175	0	1058	142	0
17	U	699	0	303	45	0
18	R	308	0	127	4	0
All	All	23364	0	22278	1620	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

The worst 5 of 1620 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:145:ARG:HH12	17:U:308:LYS:CB	1.13	1.56
8:P:165:MET:HE1	8:P:168:ARG:CD	1.22	1.55
8:P:165:MET:CE	8:P:168:ARG:HD2	1.10	1.54
16:Q:145:ARG:NH1	17:U:308:LYS:CB	1.93	1.30
16:Q:254:MET:CB	18:R:96:LEU:CB	2.13	1.27

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	204/300 (68%)	176 (86%)	25 (12%)	3 (2%)	8	36
1	o	10/300 (3%)	10 (100%)	0	0	100	100
2	H	191/253 (76%)	179 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	503/756 (66%)	447 (89%)	53 (10%)	3 (1%)	21	52
4	K	224/269 (83%)	202 (90%)	19 (8%)	3 (1%)	9	38
5	L	296/344 (86%)	261 (88%)	32 (11%)	3 (1%)	12	43
6	M	166/180 (92%)	146 (88%)	20 (12%)	0	100	100
7	N	299/345 (87%)	262 (88%)	36 (12%)	1 (0%)	36	65
8	P	220/288 (76%)	195 (89%)	22 (10%)	3 (1%)	9	37
9	S	95/138 (69%)	94 (99%)	1 (1%)	0	100	100
10	T	97/561 (17%)	93 (96%)	4 (4%)	0	100	100
11	W	73/88 (83%)	72 (99%)	1 (1%)	0	100	100
12	X	72/81 (89%)	71 (99%)	1 (1%)	0	100	100
15	C	3/943 (0%)	1 (33%)	1 (33%)	1 (33%)	0	0
15	c	11/943 (1%)	6 (54%)	4 (36%)	1 (9%)	0	8
16	Q	156/274 (57%)	151 (97%)	4 (3%)	1 (1%)	21	52
17	U	136/418 (32%)	131 (96%)	5 (4%)	0	100	100
18	R	58/177 (33%)	56 (97%)	2 (3%)	0	100	100
All	All	2814/6658 (42%)	2553 (91%)	242 (9%)	19 (1%)	20	49

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	44	PRO
1	O	156	PRO
15	C	304	ILE
16	Q	100	ILE
4	K	207	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	170/263 (65%)	167 (98%)	3 (2%)	51	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	10/263 (4%)	10 (100%)	0	100	100
2	H	174/230 (76%)	172 (99%)	2 (1%)	65	73
3	I	440/691 (64%)	435 (99%)	5 (1%)	65	73
4	K	211/260 (81%)	209 (99%)	2 (1%)	70	75
5	L	268/306 (88%)	265 (99%)	3 (1%)	65	73
6	M	147/158 (93%)	145 (99%)	2 (1%)	59	70
7	N	273/317 (86%)	271 (99%)	2 (1%)	76	77
8	P	204/259 (79%)	200 (98%)	4 (2%)	48	64
9	S	86/121 (71%)	86 (100%)	0	100	100
10	T	88/461 (19%)	85 (97%)	3 (3%)	32	55
11	W	61/77 (79%)	61 (100%)	0	100	100
12	X	65/67 (97%)	64 (98%)	1 (2%)	57	68
15	C	4/875 (0%)	4 (100%)	0	100	100
15	c	12/875 (1%)	12 (100%)	0	100	100
16	Q	109/254 (43%)	107 (98%)	2 (2%)	51	67
All	All	2322/5477 (42%)	2293 (99%)	29 (1%)	61	72

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	N	69	LEU
16	Q	83	HIS
1	O	201	PHE
10	T	533	VAL
1	O	185	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
7	N	185	HIS
8	P	84	GLN
7	N	208	GLN
1	O	193	GLN
10	T	538	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

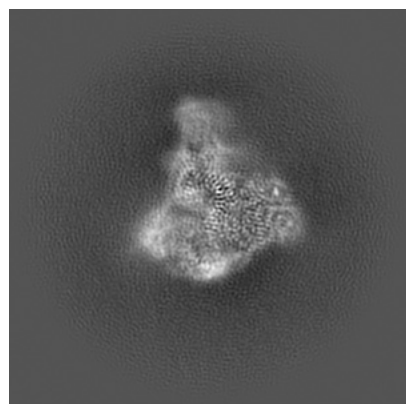
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33196. These allow visual inspection of the internal detail of the map and identification of artifacts.

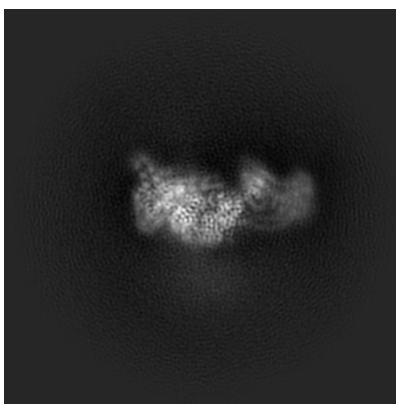
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

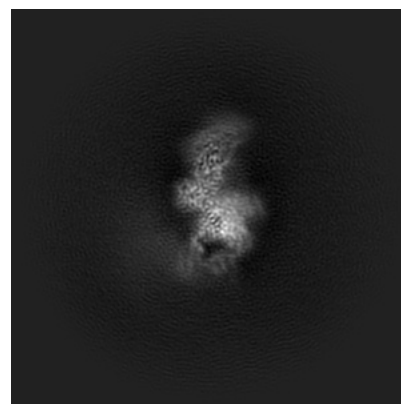
6.1.1 Primary map



X

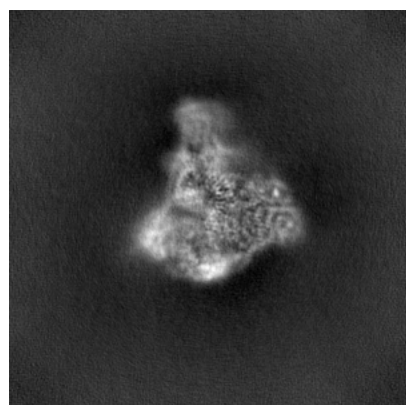


Y

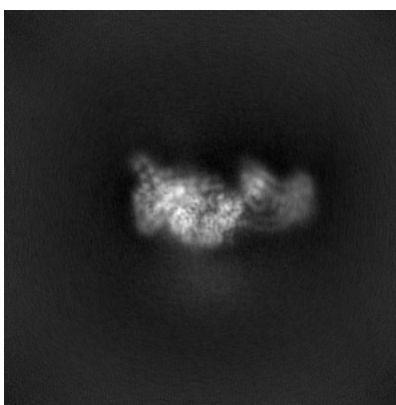


Z

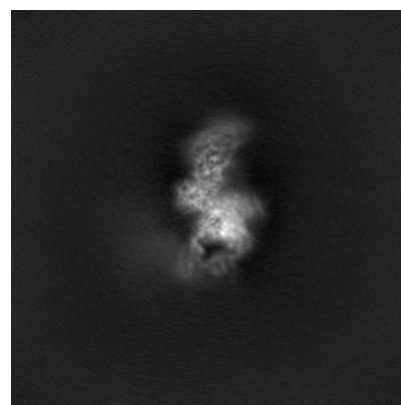
6.1.2 Raw map



X



Y

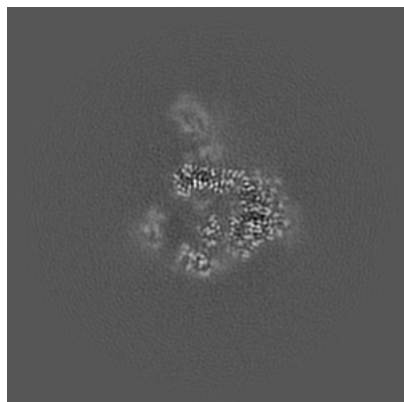


Z

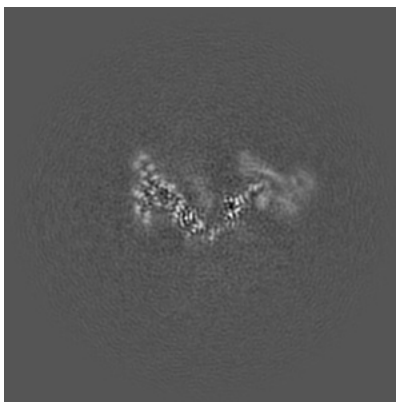
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

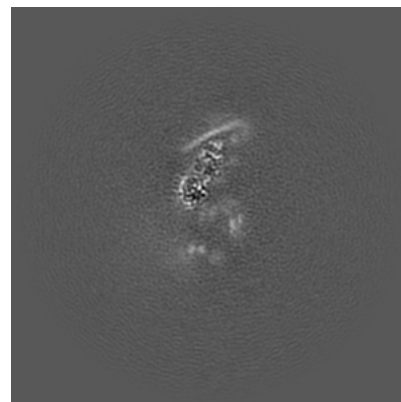
6.2.1 Primary map



X Index: 156

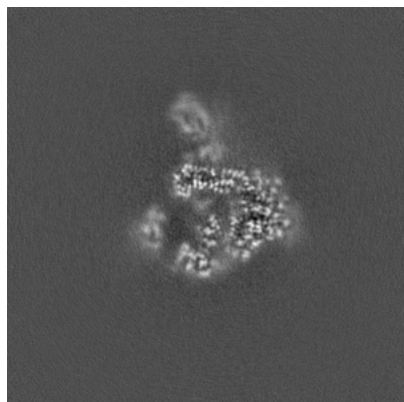


Y Index: 156

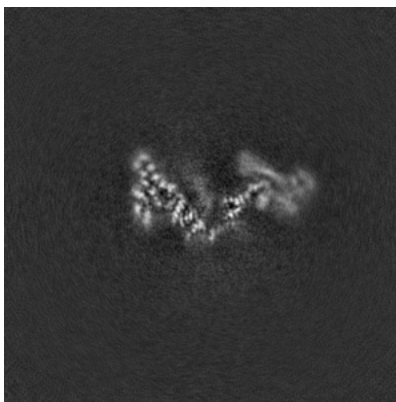


Z Index: 156

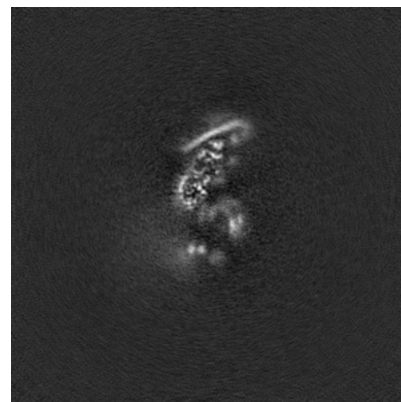
6.2.2 Raw map



X Index: 156



Y Index: 156

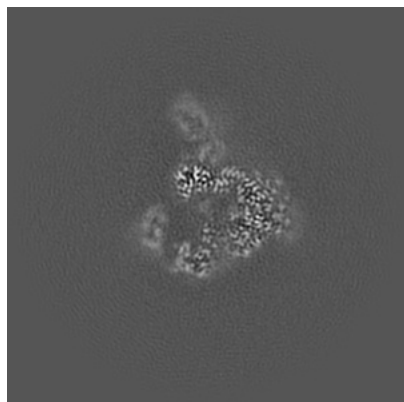


Z Index: 156

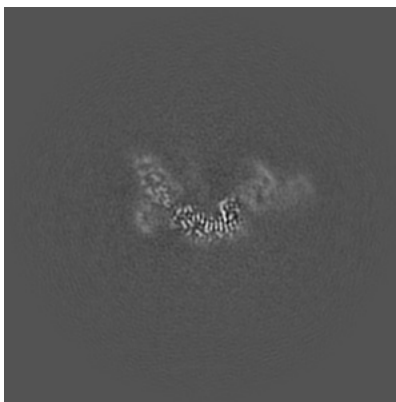
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

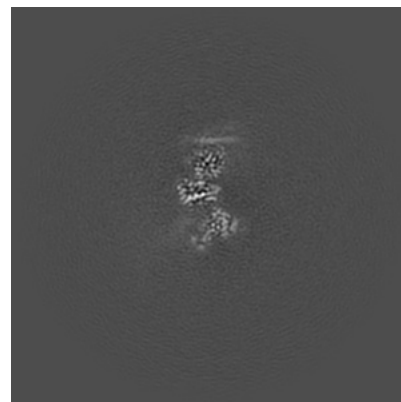
6.3.1 Primary map



X Index: 158

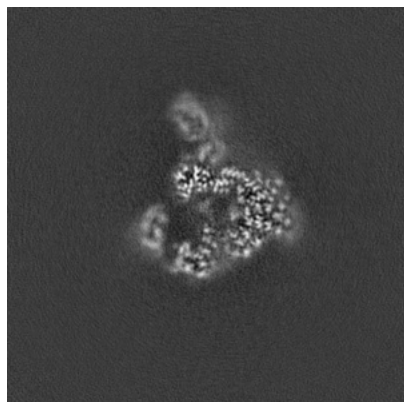


Y Index: 162

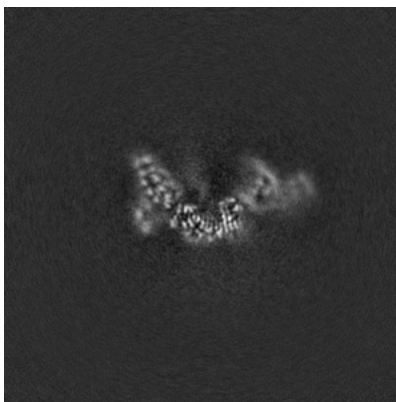


Z Index: 169

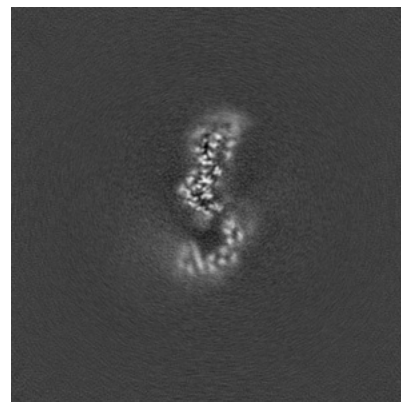
6.3.2 Raw map



X Index: 158



Y Index: 161

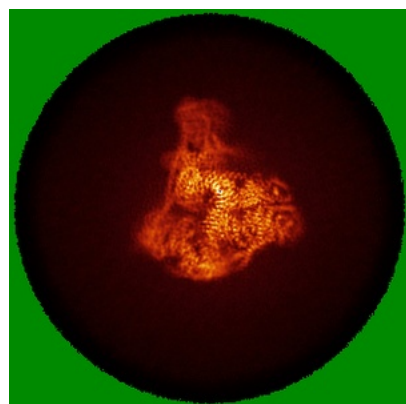


Z Index: 139

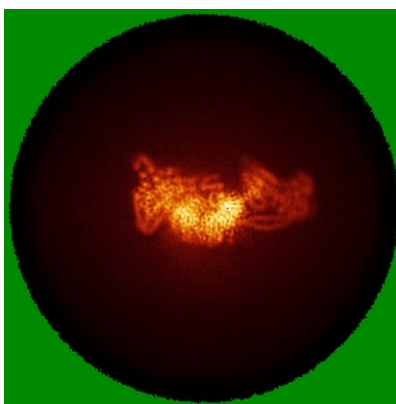
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

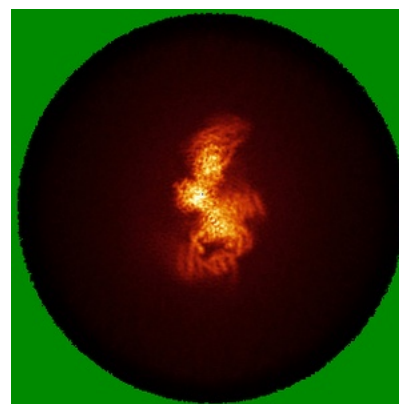
6.4.1 Primary map



X

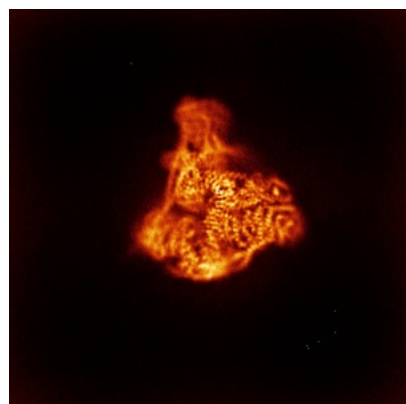


Y

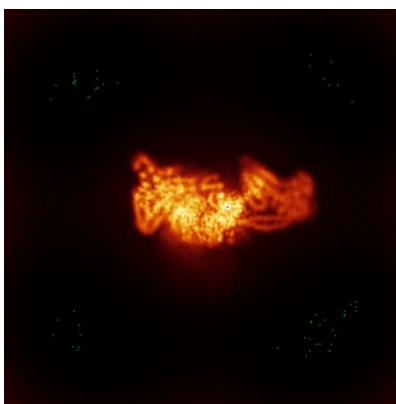


Z

6.4.2 Raw map



X



Y

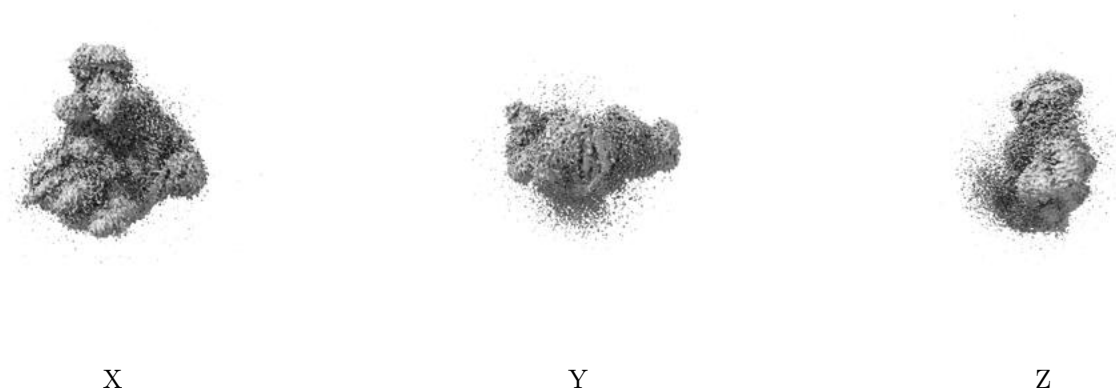


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

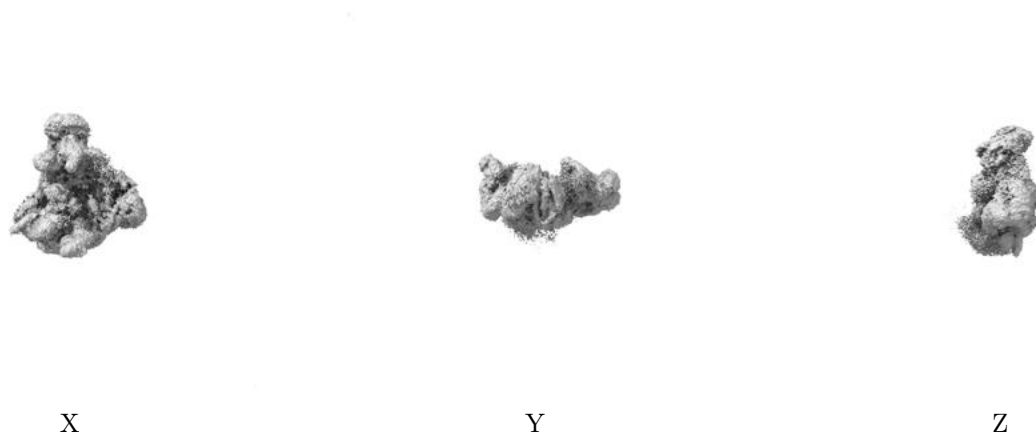
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

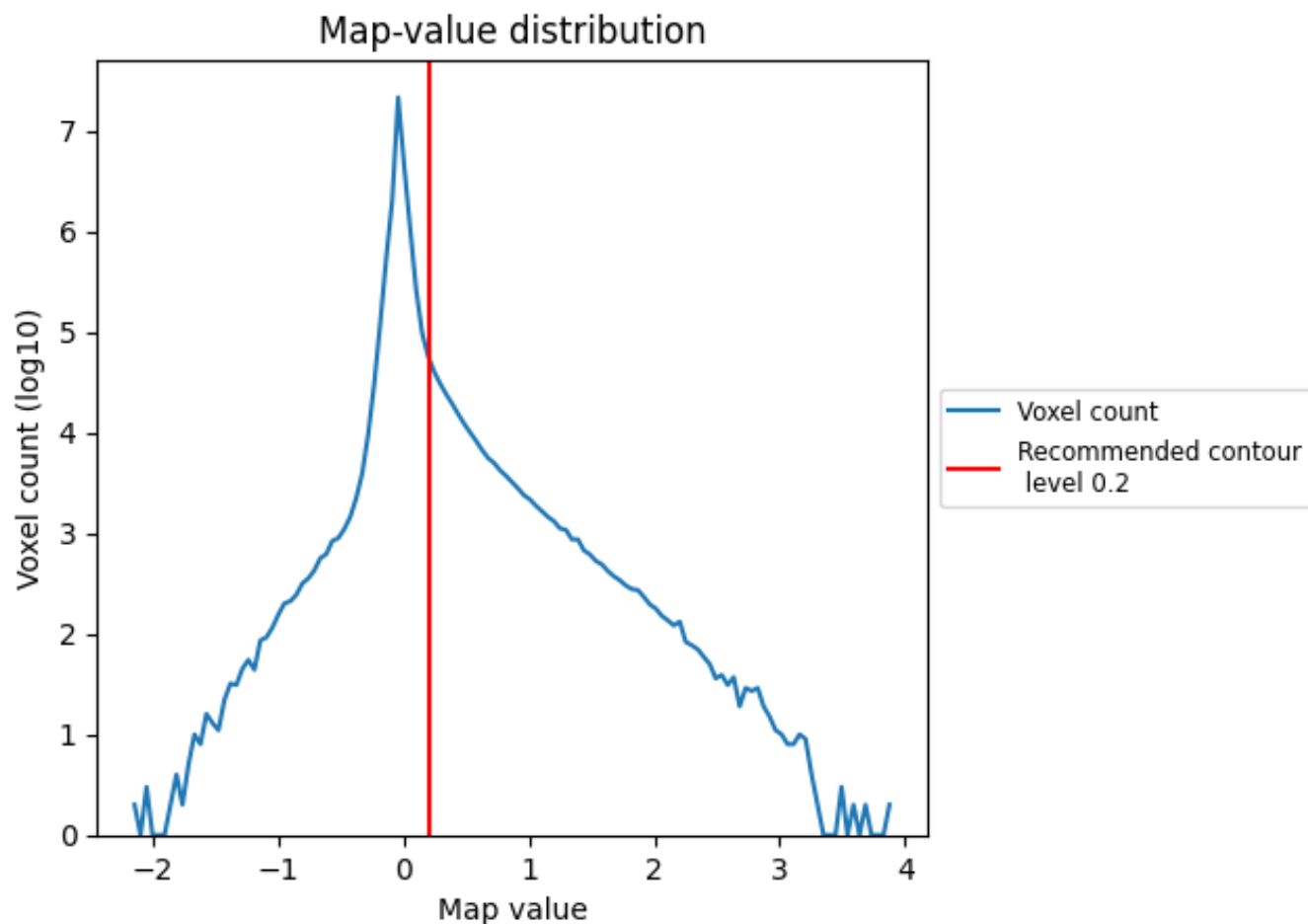
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

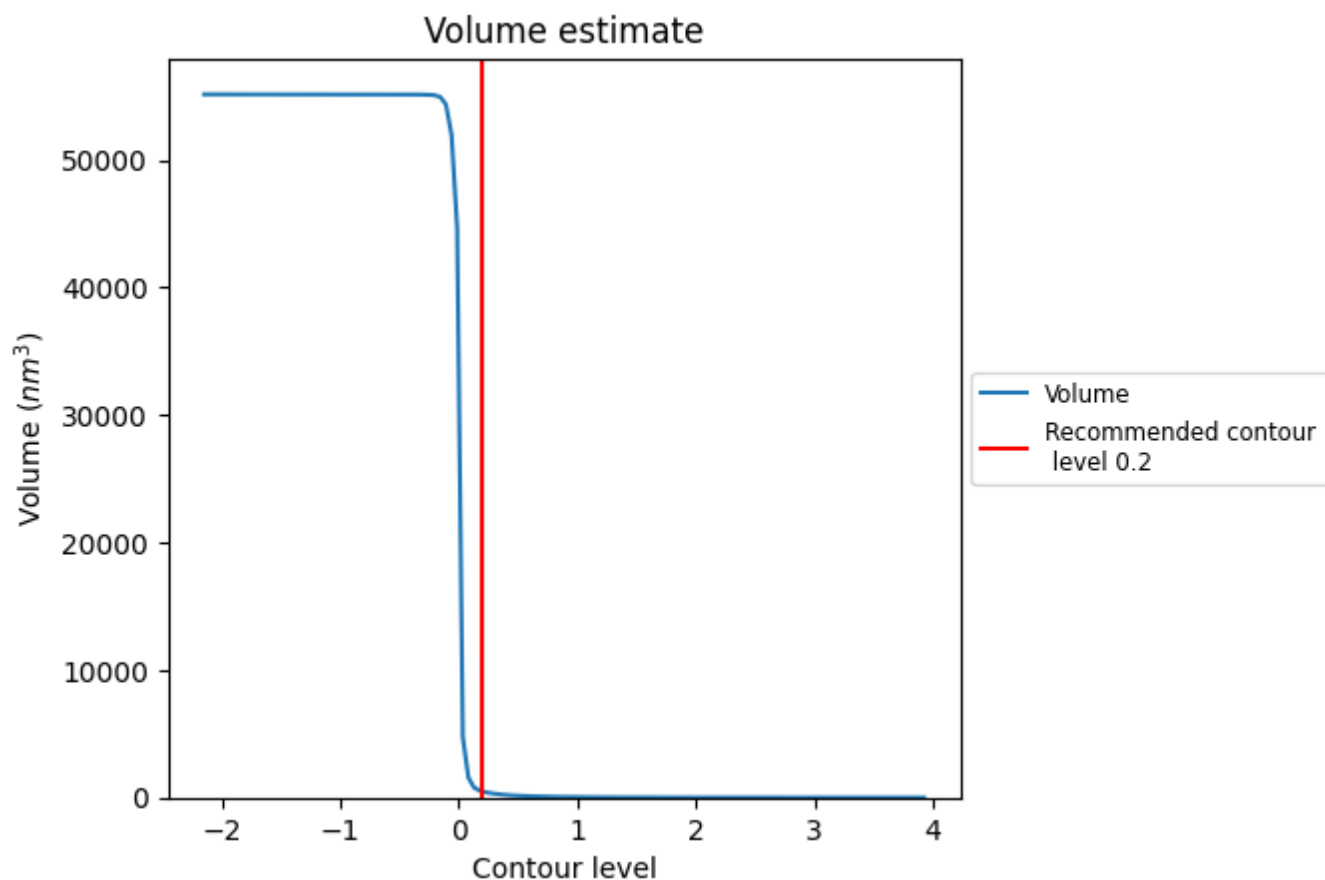
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

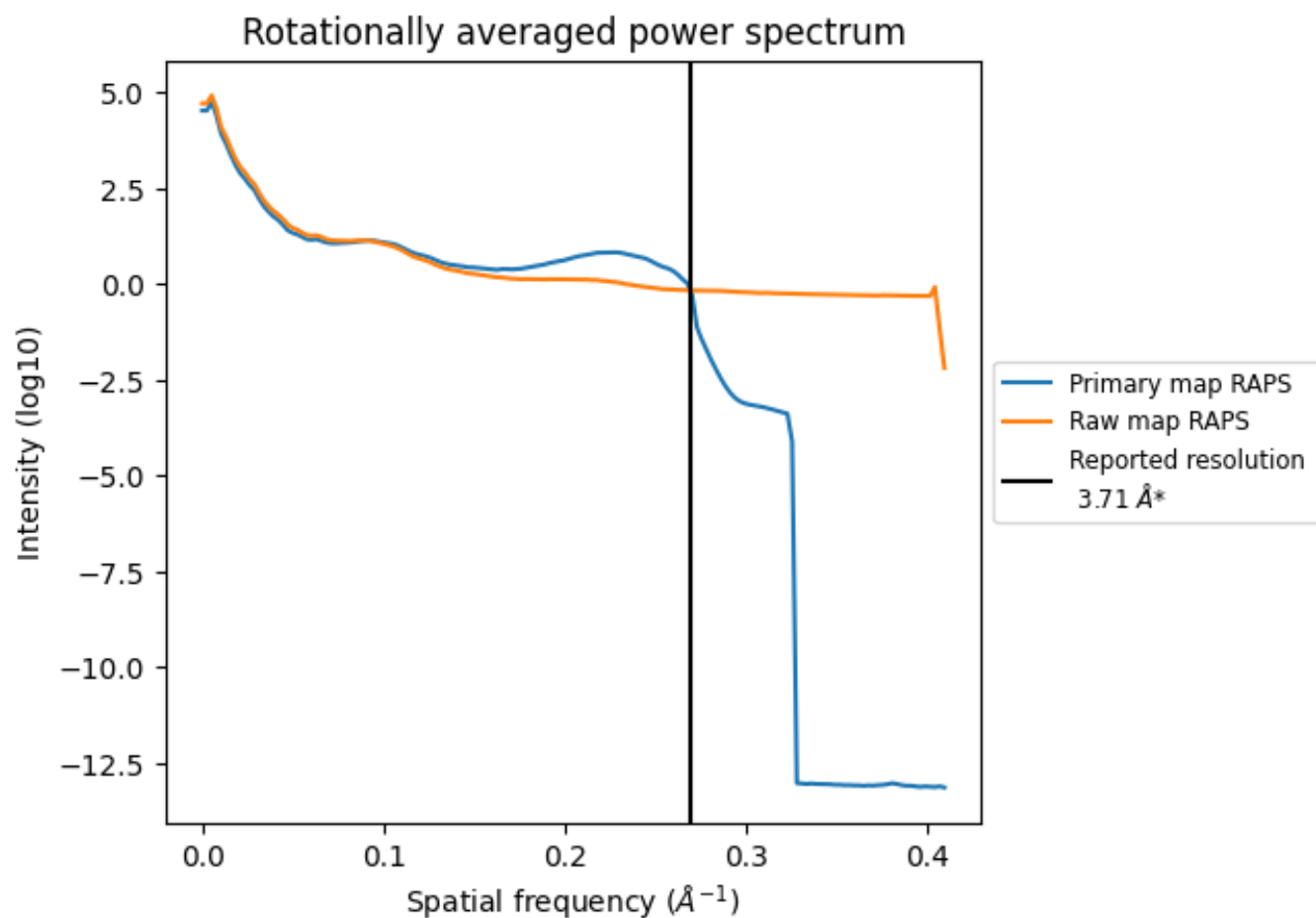
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 482 nm³; this corresponds to an approximate mass of 435 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

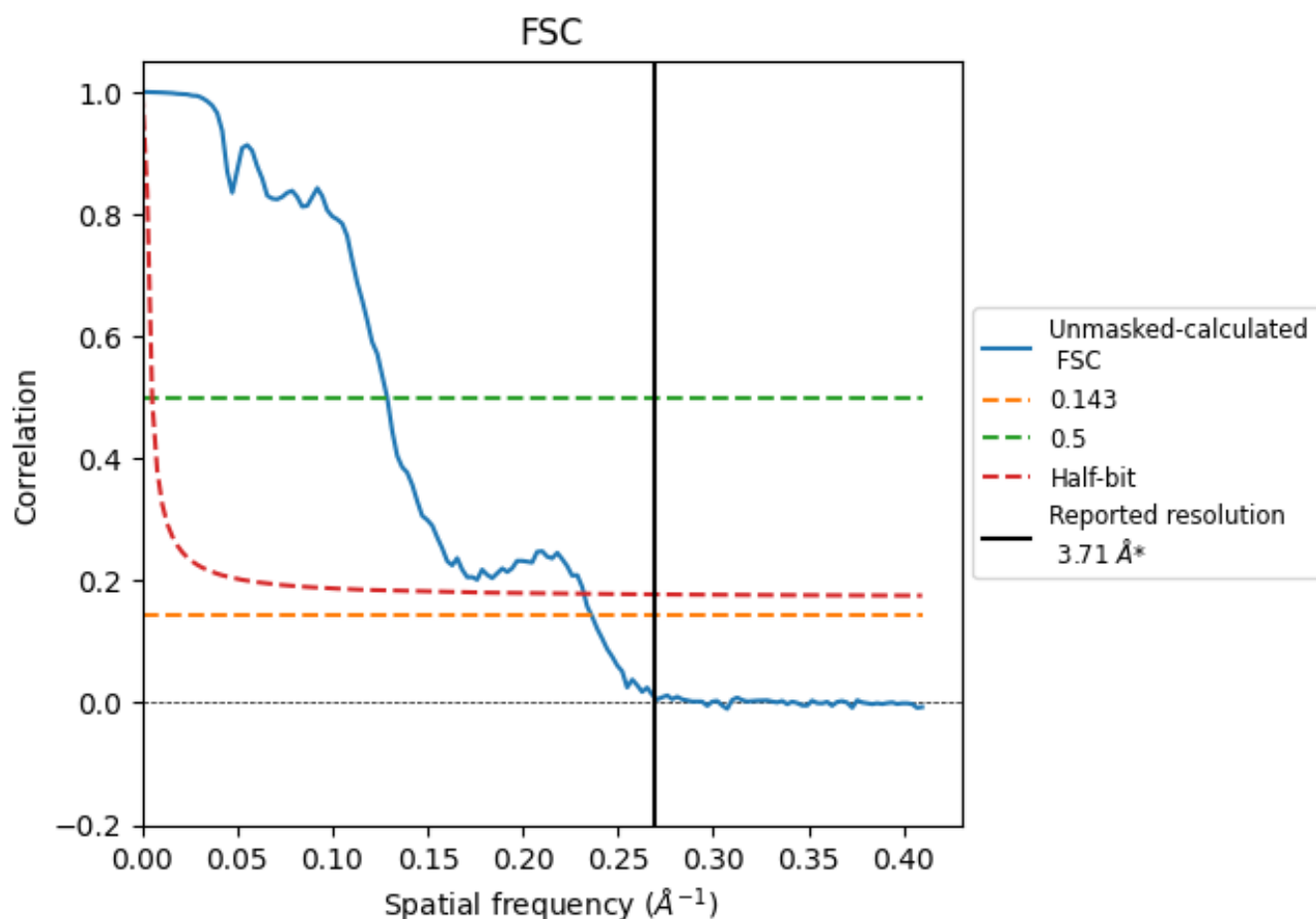


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

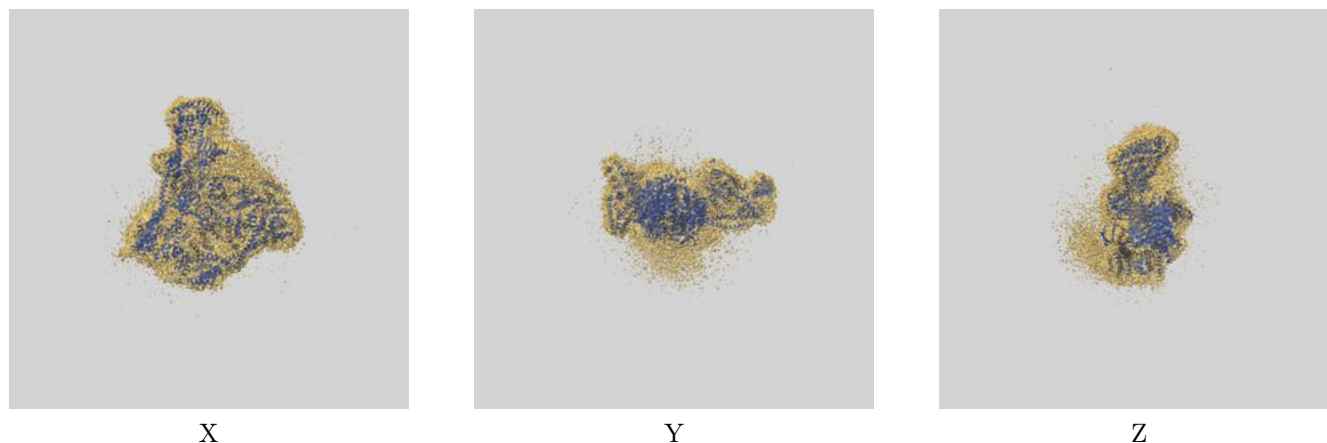
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.77	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.71 by more than 10 %

9 Map-model fit [i](#)

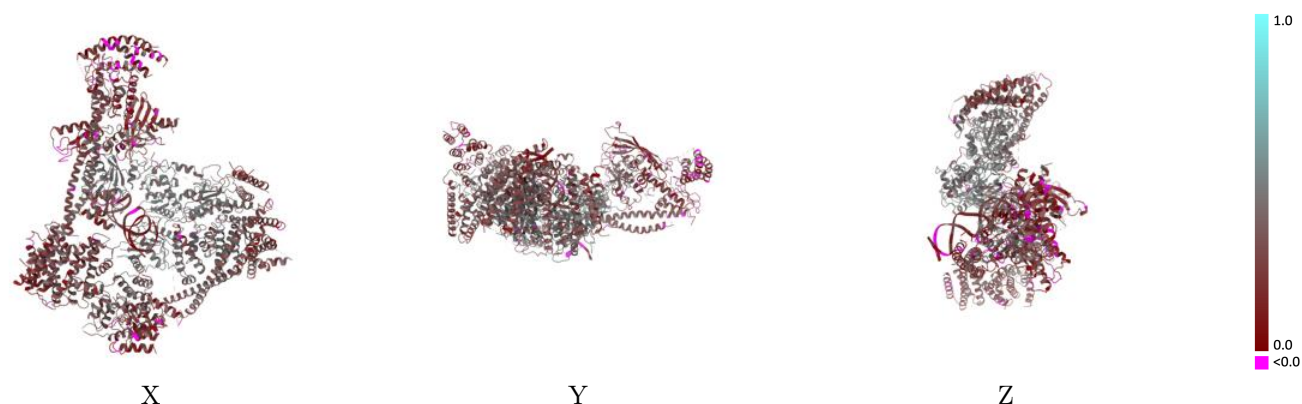
This section contains information regarding the fit between EMDB map EMD-33196 and PDB model 7XHN. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



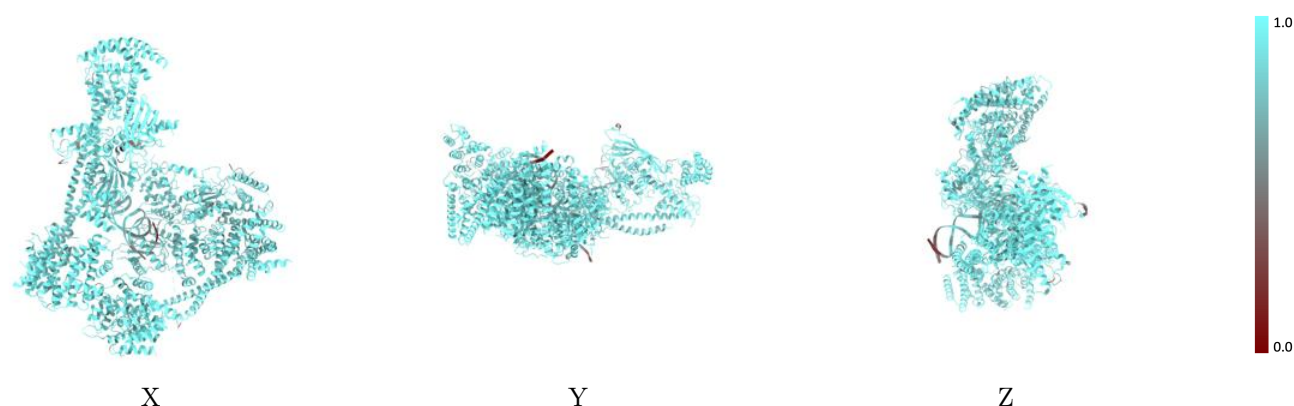
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



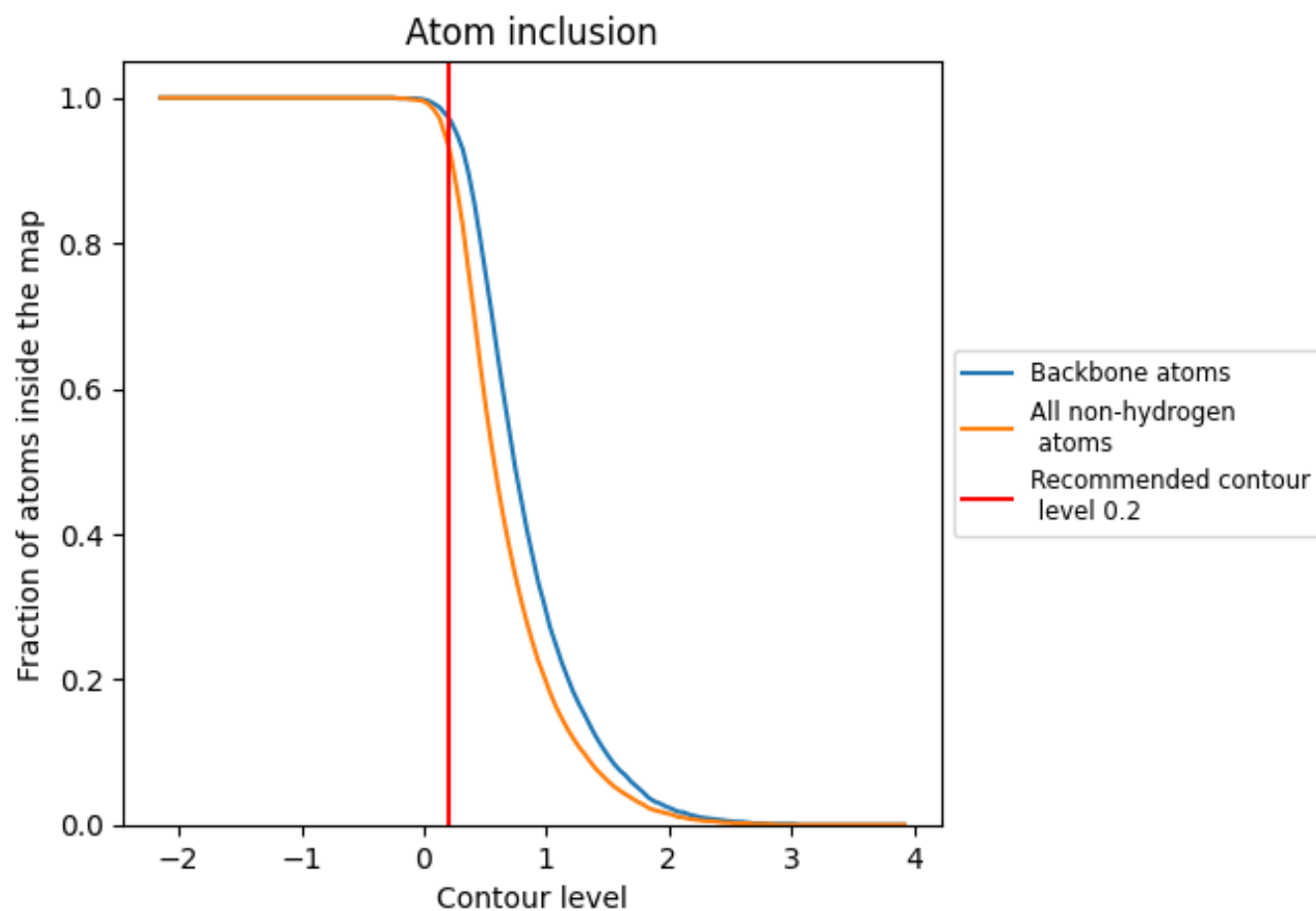
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9350	 0.3210
C	 0.8750	 0.1220
G	 0.6740	 0.1440
H	 0.9280	 0.3090
I	 0.9460	 0.3450
J	 0.6440	 0.1300
K	 0.9250	 0.3320
L	 0.9590	 0.4510
M	 0.9460	 0.4530
N	 0.9610	 0.4220
O	 0.9270	 0.2580
P	 0.9600	 0.1920
Q	 0.9540	 0.2150
R	 0.9550	 0.1730
S	 0.9650	 0.2430
T	 0.9720	 0.3410
U	 0.9990	 0.2840
W	 0.9650	 0.3230
X	 0.9150	 0.2020
c	 0.7380	 0.1720
o	 0.8820	 0.3490

